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**An *Ab Initio Study of the* Interaction between *3d* Transition Metal Atoms and Silicon Carbide Nanotubes**[1] KAPIL ADHIKARI, ASOK RAY, University of Texas at Arlington — Interaction of *3d*-transition metal atoms with armchair silicon carbide nanotubes (SiCNTs) of chiralities (3,3), (5,5), (7,7), and (9,9) is studied in detail using hybrid density functional PBE0 and an all electron basis set 6-31G**. The results show that the interaction energy between transition metal and SiCNTs depends not only on the number of *d*-electrons but also on the curvature of the nanotubes. Interaction between SiCNTs and transition metals increases with increase in curvature of the nanotubes. To explore the curvature effect in detail, both internal and external adsorption sites were chosen for the functionalization. With the exception for the SiCNTs functionalized by Ni and Zn, all 3d-transition metal-functionalized nanotubes were found to have magnetic ground states. The quenching of magnetism is strongly dependent on the curvature of the nanotubes. Mulliken charge analysis has been performed to study the amount and direction of charge transfer between transition metals and the SiCNTs. SiCNTs doped with transition metals have significantly lower band gaps, in general, than those of bare nanotubes. Transition metal atoms Ni and Zn have the least effect on the band gaps of the SiCNTs.

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